Multivariate Data Fusion and Uncertainty Quantification for Remote Sensing

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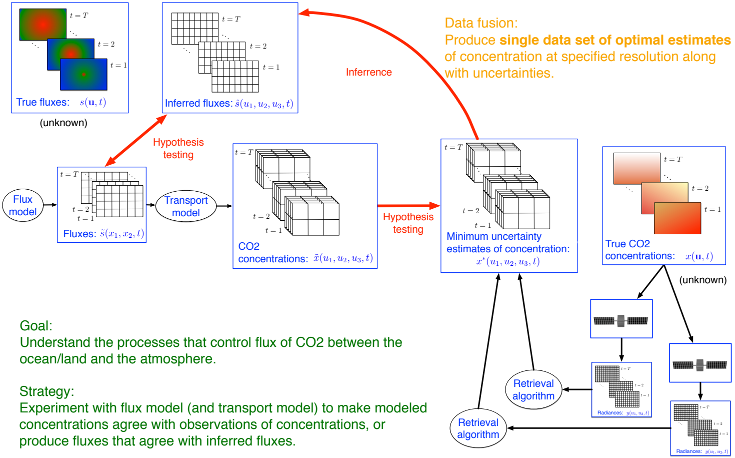
Outline

- Introduction and motivation.
- Mathematical/probabilistic framework.
- Modeling and exploiting spatial covariance.
- Modeling and exploiting temporal covariance.
- Fusing synthetic AIRS and OCO-2 profiles.
- How well did we do?
- Summary and conclusions.

Introduction and motivation



Goal:
Understand the processes that control flux of CO2 between the ocean/land and the atmosphere.

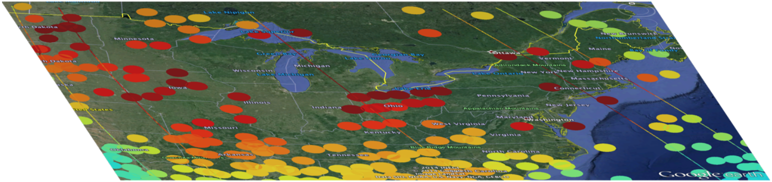
Strategy:
Experiment with flux model (and transport model) to make modeled concentrations agree with observations of concentrations, or produce fluxes that agree with inferred fluxes.

Introduction and motivation

- The goal of data fusion is to infer the values that make up a time-evolving spatial field from heterogeneous, noisy observations collected by multiple instruments.
- “Infer" = estimate the true value at any (or all) desired locations and times. Typically, this means on some grid at some pre-specified resolution.
- “Heterogeneous" = different footprints and sampling patterns.
- “Noisy" = different biases, measurement error variances, and missingness patterns.
- Exploit covariances in space, time, and among variables to make estimates with minimum uncertainty.

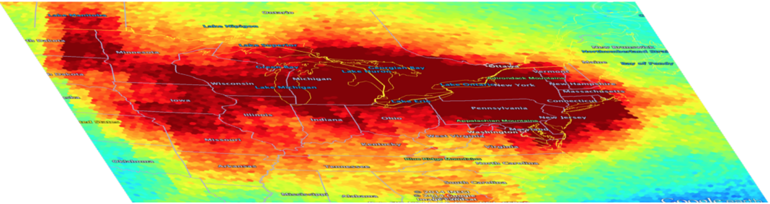
Introduction and motivation

Example: AIRS (circles) and OCO-2 (strips) synthetic data for a single time point:



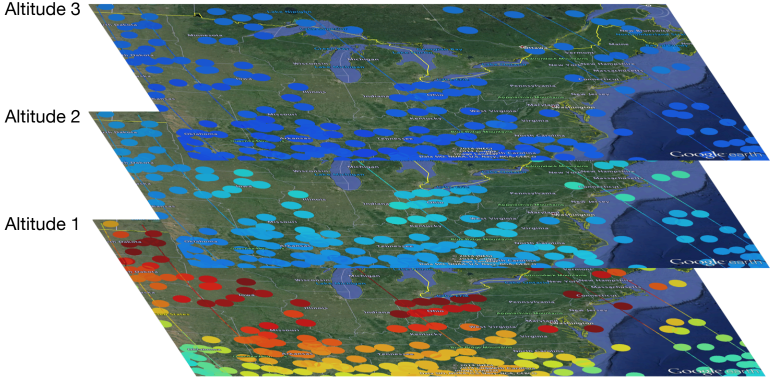
- AIRS footprints correspond to actual observed locations on January 1-3, 2006.
- OCO-2 footprints correspond to all possible observation locations (no filtering) for a single 3-day period (which one?).
- AIRS footprints = 90 km diameter. OCO-2 footprints ≈ 1 km footprints (strip = 4-across).

"True" (synthetic) field at at single time point:



- Find the estimate of the field that minimizes the uncertainty (estimate is unbiased and has minimum variance) by using all the OCO-2 and AIRS footprints to make estimates at all locations (and times!).

Introduction and motivation



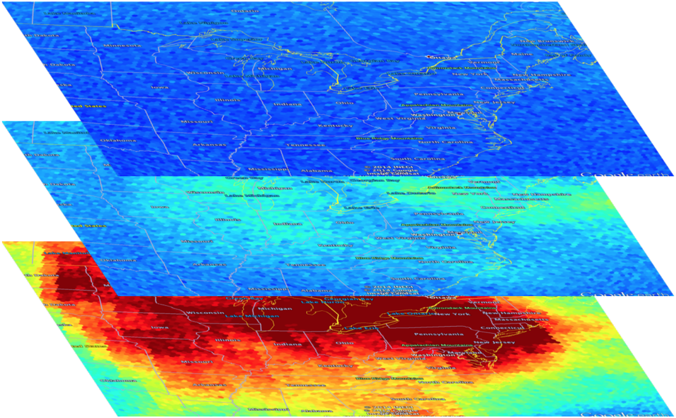
Multivariate data fusion: estimate vector-valued quantities, e.g., vertical profiles of CO2 mole-fraction.

Introduction and motivation

Altitude 3

Altitude 2

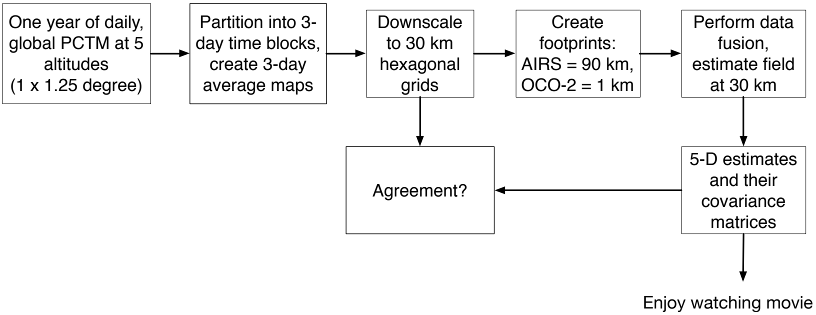
Altitude 1



- Find the minimum uncertainty estimate of the *multivariate* field using all the OCO-2 and AIRS observed profiles to make estimates at all locations, altitudes, and times.

Fusing synthetic AIRS and OCO-2 profiles

Fuse one year of synthetic AIRS and OCO-2 five-altitude profiles:

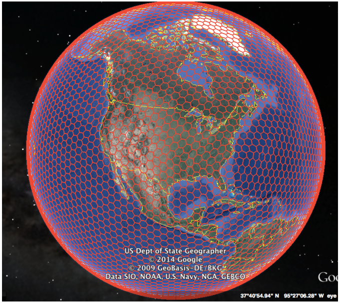


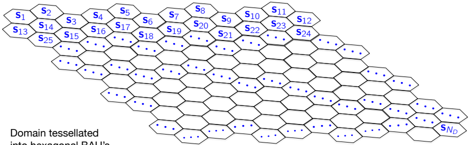
Fusing synthetic AIRS and OCO-2 profiles

Fused estimate, near surface CO2 mole-fraction (ppm):

Click me.

Mathematical/probabilistic framework





Domain tessellated into hexagonal BAU's

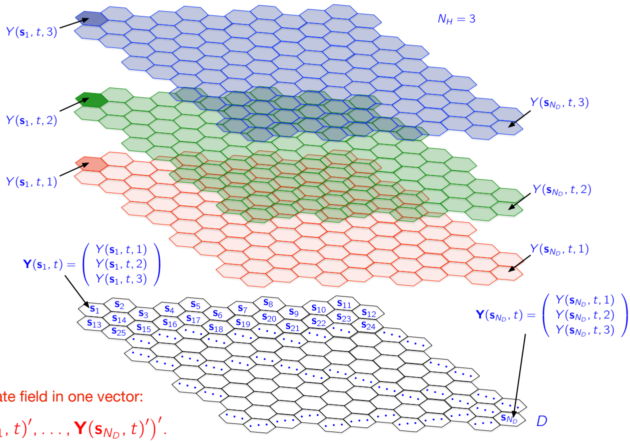
- Partition of Earth's surface into N_D (D is for "domain"), small hexagonal basic areal units (BAU's; 30 km in our application); the same at all time steps.
- BAU's indexed by **s**=lat/lon of their centers.
- Partition time into three-day blocks (basic time unit, BTU), indexed by t.
- At each BAU-BTU combination, there is a true but not directly observed vertical profile of CO2 mole-fraction,

$$\mathbf{Y}(\mathbf{s}, t) = (Y(\mathbf{s}, t, 1), \ldots, Y(\mathbf{s}, t, N_H))',$$

where N_H = number of altitudes.

Mathematical/probabilistic framework

Geophysical field:

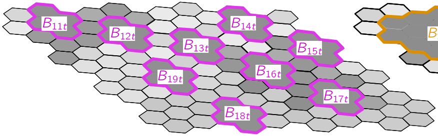


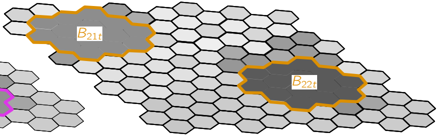
The whole multivariate field in one vector:

$$\mathbf{Y}_t = \left(\mathbf{Y}(\mathbf{s}_1, t)', \ldots, \mathbf{Y}(\mathbf{s}_{N_D}, t)'\right)'.$$

Mathematical/probabilistic framework

Observations are the averages of BAU values within instrument footprints, plus footprint-level measurement error.





$$\mathbf{Z}^{(1)}(B_{1it}) = \frac{1}{|D \cap B_{1it}|} \sum_{\mathbf{s} \in D \cap B_{1it}} \mathbf{Y}(\mathbf{s}, t) + \boldsymbol{\epsilon}(B_{1it})$$

$$\mathbf{Z}^{(2)}(B_{2jt}) = \frac{1}{|D \cap B_{2jt}|} \sum_{\mathbf{s} \in D \cap B_{2jt}} \mathbf{Y}(\mathbf{s}, t) + \boldsymbol{\epsilon}(B_{2jt})$$

All instrument 1 observations in one vector:

$$\mathbf{Z}_t^{(1)} = \left(\mathbf{Z}^{(1)}(B_{11t})', \ldots, \mathbf{Z}^{(1)}(B_{1N_t^{(1)}t})'\right)'$$

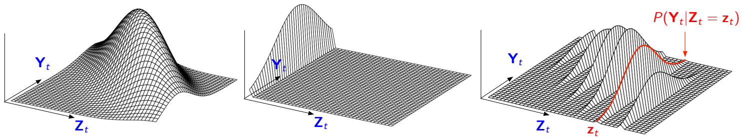
All instrument 2 observations in one vector:

$$\mathbf{Z}_t^{(2)} = \left(\mathbf{Z}^{(2)}(B_{21t})', \ldots, \mathbf{Z}^{(2)}(B_{1N_t^{(2)}t})'\right)'$$

All observations in one vector: $\mathbf{Z}_t = \left(\mathbf{Z}_t^{(1)\prime}, \mathbf{Z}_t^{(2)\prime}\right)'$.

Mathematical/probabilistic framework

- $\mathbf{Z}_t$ is the vector of all “noisy" observations (measurement and aggregation error).
- $\mathbf{Y}_t$ is the vector of all unknown (uncertain and not directly observed) values of the high-resolution spatial field.
- We want to estimate $\mathbf{Y}_t$ given $\mathbf{Z}_t$.

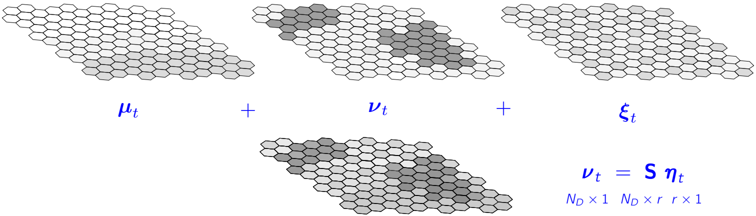


- The minimum uncertainty (unbiased, minimum variance) estimate of $\mathbf{Y}_t$ given the observed data, $\mathbf{Z}_t$, is $\mathrm{E}(\mathbf{Y}_t|\mathbf{Z}_t)$. The uncertainty is $\mathrm{var}(\mathbf{Y}_t|\mathbf{Z}_t)$. (Expected value and covariance matrix of the posterior distribution of $\mathbf{Y}_t$ given $\mathbf{Z}_t$.)

Modeling and exploiting spatial covariance

Strategy: break $\mathbf{Y}_t$ into pieces, estimate pieces separately.

trend | small-scale variation | fine-scale variation



$$\boldsymbol{\mu}_t \quad + \quad \boldsymbol{\nu}_t \quad + \quad \boldsymbol{\xi}_t$$

$$\mathbf{Y}_t$$

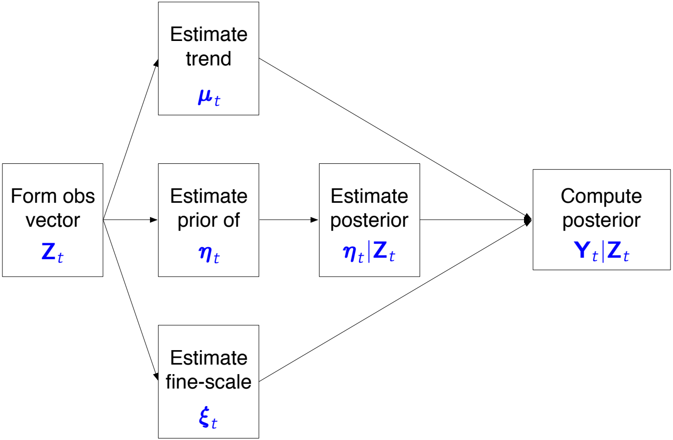
$$\underset{N_D \times 1}{\boldsymbol{\nu}_t} = \underset{N_D \times r}{\mathbf{S}} \; \underset{r \times 1}{\boldsymbol{\eta}_t}$$

$\mathbf{S}$ = matrix of spatial basis functions
$\boldsymbol{\eta}_t$ = coefficients

The field $\mathbf{Y}_t$ is the super-position of three independent components: the trend, $\boldsymbol{\mu}_t$, the small-scale variation, $\boldsymbol{\nu}_t$, and the fine-scale variation, $\boldsymbol{\xi}_t$. Write

$$\mathbf{Y}_t = \boldsymbol{\mu}_t + \boldsymbol{\nu}_t + \boldsymbol{\xi}_t, \quad \text{and} \quad \mathrm{E}(\mathbf{Y}_t|\mathbf{Z}_t) = \mathrm{E}(\boldsymbol{\mu}_t|\mathbf{Z}_t) + \mathbf{S}\,\mathrm{E}(\boldsymbol{\eta}_t|\mathbf{Z}_t) + \mathrm{E}(\boldsymbol{\xi}_t|\mathbf{Z}_t),$$
$$\mathrm{cov}(\mathbf{Y}_t|\mathbf{Z}_t) = \mathrm{cov}(\boldsymbol{\mu}_t|\mathbf{Z}_t) + \mathbf{S}\,\mathrm{cov}(\boldsymbol{\eta}_t|\mathbf{Z}_t)\,\mathbf{S}' + \mathrm{cov}(\boldsymbol{\xi}_t|\mathbf{Z}_t).$$

Modeling and exploiting spatial covariance

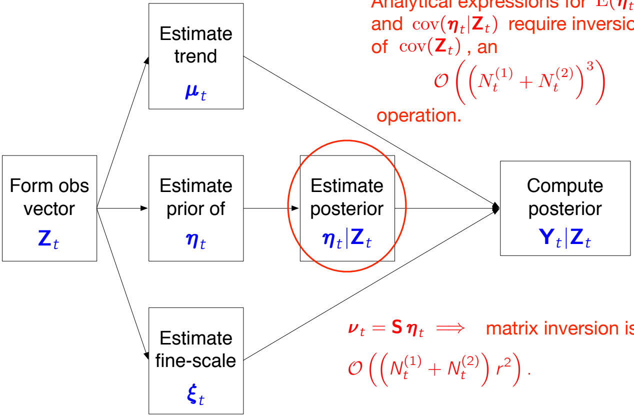


Modeling and exploiting spatial covariance

Analytical expressions for $\mathrm{E}(\boldsymbol{\eta}_t|\mathbf{Z}_t)$ and $\mathrm{cov}(\boldsymbol{\eta}_t|\mathbf{Z}_t)$ require inversion of $\mathrm{cov}(\mathbf{Z}_t)$, an

$$\mathcal{O}\left(\left(N_t^{(1)} + N_t^{(2)}\right)^3\right)$$

operation.



$\boldsymbol{\nu}_t = \mathbf{S}\,\boldsymbol{\eta}_t \implies$ matrix inversion is

$$\mathcal{O}\left(\left(N_t^{(1)} + N_t^{(2)}\right) r^2\right).$$

Modeling and exploiting temporal covariance

Apply Kalman Smoother to $\boldsymbol{\eta}_t$ (Nguyen et al., 2013):

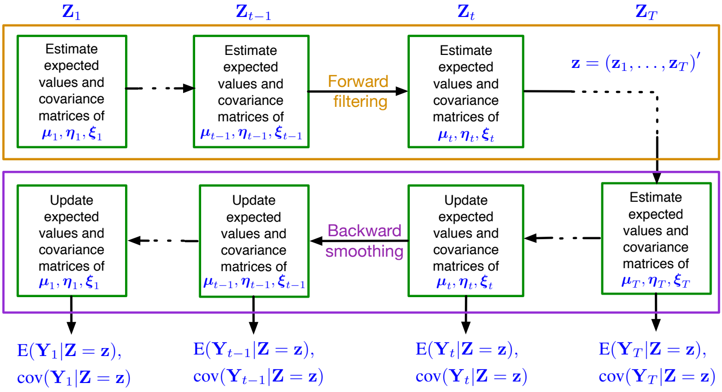
- Model the temporal evolution of $\boldsymbol{\eta}_t$ as an auto-regressive process:

$$\boldsymbol{\eta}_{t+1} = \mathbf{H}\boldsymbol{\eta}_t + \boldsymbol{\zeta}_t, \quad \boldsymbol{\zeta}_t \sim N(\mathbf{0}, \mathbf{U}),$$

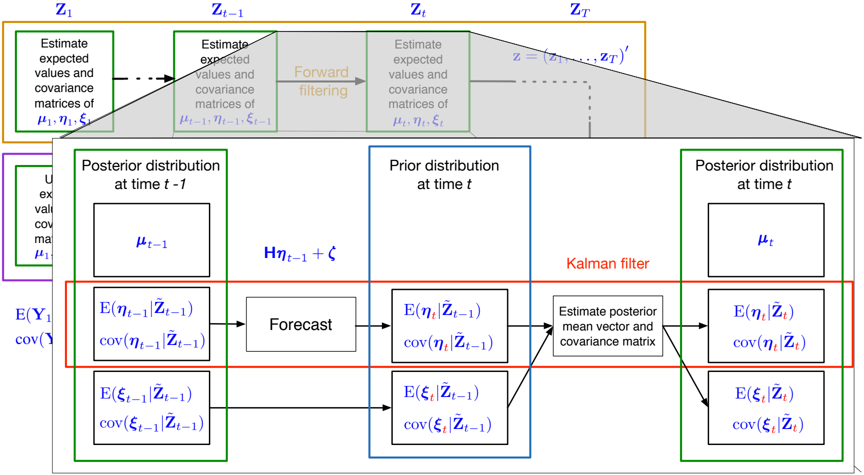
  where $\mathbf{H}$ is the "propagator" matrix, and $\boldsymbol{\zeta}_t$ is the "innovation" matrix.

- Estimate $\mathbf{H}$ and $\mathbf{U}$ from the observations.
- Forward filtering: for each time block (BTU) $t = 1, \ldots, T$, obtain maximum likelihood estimates (via the EM algorithm) of the parameters of posterior distribution of $\boldsymbol{\eta}_t$.
- Backward smoothing: for each time block, filter backwards in time so that the estimates are based on *all* data from all time blocks.

Modeling and exploiting temporal covariance



Modeling and exploiting temporal covariance



$$\tilde{\mathbf{Z}}_t = (\mathbf{Z}_t, \mathbf{Z}_{t-1}, \ldots, \mathbf{Z}_1)\,.$$

Fusing synthetic AIRS and OCO-2 profiles

Fuse one year of synthetic AIRS and OCO-2 five-altitude profiles:

- Synthetic truth field (five altitudes) created by downscaling output of the Parameterized Chemistry Transport Model (PCTM).
  - 365 daily model runs at $1^\circ \times 1.25^\circ$ resolution.
  - Downscaled to 30 km resolution using conditional simulation (Stough et al., 2014).
- Synthetic AIRS footprints (90 km) obtained by averaging 30 km hexagons belonging to actual AIRS footprints for corresponding day of 2006 (cloud-screened).
- Synthetic OCO-2 footprints ($\approx$ 1 km) obtained as value of 30 km hexagon to which footprint center belongs for representative orbit tracks (not cloud-screened).
- No measurement error (yet).

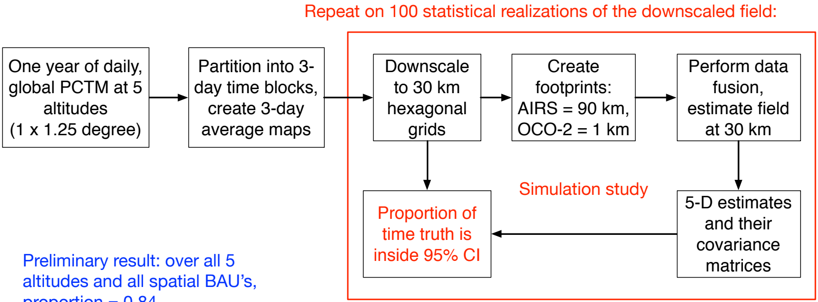
Fusing synthetic AIRS and OCO-2 profiles

Fuse one year of synthetic AIRS and OCO-2 five-altitude profiles:

- Time aggregated into three-day blocks, Kalman smoother run on monthly "windows" (ten three-day blocks per month). Propagator matrix and innovation vector re-estimated for each window.
- About 40,000 AIRS and 200,000 OCO-2 synthetic observations per three-day block.
- We used $r \approx 1800$ basis centers in three dimensions (300 horizontal $\times$ 6 vertical at each horizontal location).
- Estimated five-altitude profile and their covariance matrices produced at 30 km BAU resolution globally for 120, three-day time blocks covering one (synthetic) year.
- Timing: fusing one month (five altitudes) in ten, three-day blocks takes about 36 hours on a single Intel Xeon 2.0 Ghz processor.

How well did we do?

Fuse one year of synthetic AIRS and OCO-2 five-altitude profiles:



Preliminary result: over all 5 altitudes and all spatial BAU's, proportion = 0.84.

Summary and conclusions

- Spatial (and inter-variable) dependence captured by a combination of basis functions and a low-dimensional hidden state vector. Estimation performed in low-dimensional space. No assumptions of isotropy or stationarity required.
- Temporal dependence via a Kalman smoother on the hidden state.
- Corrects for change of support (heterogenous footprints) and different measurement error characteristics.
- Computationally feasible for very large remote sensing data sets.
- *No instrument observes everywhere all the time, or perfectly. Here we leverage complementary strengths of multiple instruments to increase coverage and minimize uncertainty.*

Summary and conclusions

- Still work to do in evaluating results through simulation studies.
- Still work to do on the selection of basis functions and interplay between them, the trend, and the fine-scale term.
- Preparing to apply to actual AIRS and OCO-2 data early next year.
- Journal paper in preparation.

References

Nguyen, H., Cressie, N., and Braverman, A. (2012). Spatial Statistical Data Fusion for Remote- Sensing Applications, *Journal of the American Statistical Association*, 107, pp. 1004-1018.

Nguyen, H., Katzfuss, M., Cressie, N., and Braverman, A. (2013). Spatio-Temporal Data Fusion for Very Large Remote Sensing Datasets, *Technometrics*, DOI: 10.1080/00401706.2013.831774.

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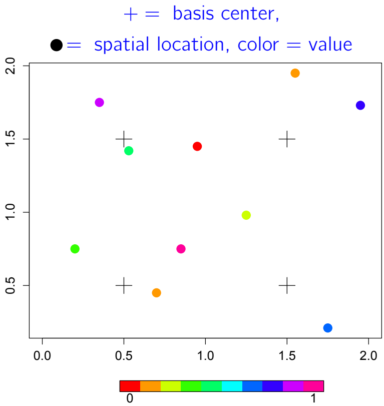
Backup slides

Spatial basis functions

2-D cartoon example, 10 locations, 4 basis centers:



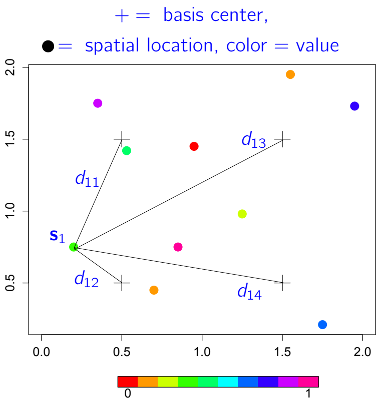
Spatial structure given by $\mathrm{cov}(\boldsymbol{\nu}_t)$.

10×10

$$\boldsymbol{\nu}_t = (\nu(\mathbf{s}_1, t), \ldots, \nu(\mathbf{s}_{10}, t))'$$

Spatial basis functions

2-D cartoon example, 10 locations, 4 basis centers:



Basis function for each location is a decaying function of its distance to the four basis centers:

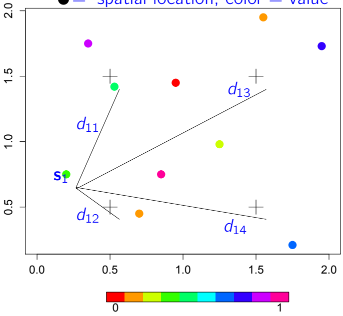
$$\mathbf{S}(\mathbf{s}_1) = (1/d_{11}, 1/d_{12}, 1/d_{13}, 1/d_{14})\,.$$

Spatial basis functions

2-D cartoon example, 10 locations, 4 basis centers:

$+ =$ basis center,

$\bullet =$ spatial location, color $=$ value



$\boldsymbol{\nu}_t$

Basis function matrix:

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}(\mathbf{s}_1) \\ \mathbf{S}(\mathbf{s}_2) \\ \vdots \\ \mathbf{S}(\mathbf{s}_{10}) \end{pmatrix} = \begin{pmatrix} 1/d_{11} & 1/d_{12} & 1/d_{13} & 1/d_{14} \\ 1/d_{21} & 1/d_{22} & 1/d_{23} & 1/d_{24} \\ \vdots & \vdots & \vdots & \vdots \\ 1/d_{10,1} & 1/d_{10,2} & 1/d_{10,3} & 1/d_{10,4} \end{pmatrix}$$

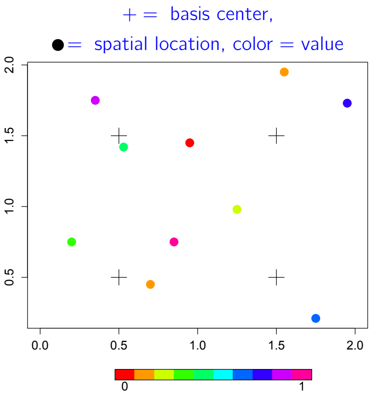
Low-dimensional representation:

$$\mathbf{S}\,\boldsymbol{\eta}_t = \begin{pmatrix} 1/d_{11} & 1/d_{12} & 1/d_{13} & 1/d_{14} \\ 1/d_{21} & 1/d_{22} & 1/d_{23} & 1/d_{24} \\ \vdots & \vdots & \vdots & \vdots \\ 1/d_{10,1} & 1/d_{10,2} & 1/d_{10,3} & 1/d_{10,4} \end{pmatrix} \begin{pmatrix} \eta_{1t} \\ \eta_{2t} \\ \eta_{3t} \\ \eta_{4t} \end{pmatrix}$$

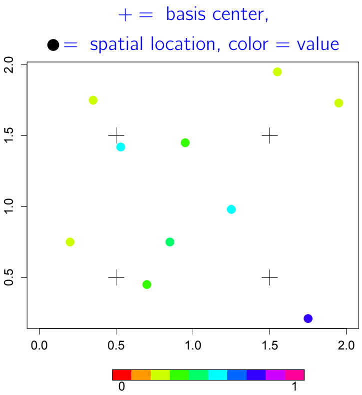
$$\mathrm{cov}(\boldsymbol{\nu}_t) = \mathrm{cov}(\mathbf{S}\,\boldsymbol{\eta}_t) = \mathbf{S}\,\underbrace{\mathrm{cov}(\boldsymbol{\eta}_t)}_{4 \times 4}\,\mathbf{S}'$$

Spatial basis functions

2-D cartoon example, 10 locations, 4 basis centers:



$\boldsymbol{\nu}_t$



$\hat{\boldsymbol{\nu}}_t = \mathbf{S}\,\hat{\boldsymbol{\eta}}_t.$

Modeling and exploiting spatial covariance

- Have $P(\mathbf{Z}_t|\boldsymbol{\eta}_t)$, want $P(\boldsymbol{\eta}_t|\mathbf{Z}_t)$. Use Bayes' Theorem $(P(B|A) \propto P(A|B)P(B).)$

$$\mathbf{Y}(\mathbf{s}, t) = \boldsymbol{\mu}(\mathbf{s}, t) + \boldsymbol{\nu}(\mathbf{s}, t) + \boldsymbol{\xi}(\mathbf{s}, t)$$

$$\swarrow \qquad \searrow$$

$$\mathbf{Z}^{(1)}(B_{1it}) = \frac{1}{|D \cap B_{1it}|} \sum_{s \in B_{1it}} \mathbf{Y}(\mathbf{s}, t) + \boldsymbol{\epsilon}(B_{1it}) \qquad \mathbf{Z}^{(2)}(B_{2jt}) = \frac{1}{|D \cap B_{2jt}|} \sum_{s \in B_{2jt}} \mathbf{Y}(\mathbf{s}, t) + \boldsymbol{\epsilon}(B_{2jt})$$

$$\mathbf{Z}_t^{(1)} = \boldsymbol{\mu}_t^{(1)} + \mathbf{S}^{(1)}\boldsymbol{\eta}_t^{(1)} + \boldsymbol{\xi}_t^{(1)} + \boldsymbol{\epsilon}_t^{(1)} \qquad \mathbf{Z}_t^{(2)} = \boldsymbol{\mu}_t^{(2)} + \mathbf{S}^{(2)}\boldsymbol{\eta}_t^{(2)} + \boldsymbol{\xi}_t^{(2)} + \boldsymbol{\epsilon}_t^{(2)}$$

$$\searrow \qquad \swarrow$$

$$\begin{pmatrix} \mathbf{Z}_t^{(1)} \\ \mathbf{Z}_t^{(2)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\mu}_t^{(1)} \\ \boldsymbol{\mu}_t^{(2)} \end{pmatrix} + \begin{pmatrix} \mathbf{S}_t^{(1)} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}_t^{(2)} \end{pmatrix} \begin{pmatrix} \boldsymbol{\eta}_t^{(1)} \\ \boldsymbol{\eta}_t^{(2)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\xi}_t^{(1)} \\ \boldsymbol{\xi}_t^{(2)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{\epsilon}_t^{(1)} \\ \boldsymbol{\epsilon}_t^{(2)} \end{pmatrix}$$

$$\Downarrow$$

$$\mathbf{Z}_t = \boldsymbol{\mu}_t + \mathbf{S}\,\boldsymbol{\eta}_t + \boldsymbol{\xi}_t + \boldsymbol{\epsilon}_t$$

- $P(\boldsymbol{\eta}_t|\mathbf{Z}_t) \propto P(\mathbf{Z}_t|\boldsymbol{\eta}_t)P(\boldsymbol{\eta}_t)$.

Vertical basis functions

- In previous work (Nguyen, Katzfuss, Cressie, and Braverman (2012)) we used 446 basis centers arranged in a multi-resolution configuration with local bisquare decay to capture 2-D spatial structure in $\boldsymbol{\nu}_t$.

- Basis functions for 3-D location$(\mathbf{s}, h)$ is $\mathcal{S}(\mathbf{s}, h)$. It is the Kronecker product of the horizontal basis function, $\mathbf{S}(\mathbf{s})$, and vertical (horizontally varying) basis function $\boldsymbol{\tau}(\mathbf{s}, h)$:

$$\mathcal{S}(\mathbf{s}, h) = \mathbf{S}(\mathbf{s}) \otimes \boldsymbol{\tau}(\mathbf{s}, h).$$

Example:

$$\mathbf{S}(\mathbf{s}) = \begin{pmatrix} S_1 \\ \vdots \\ S_{r_1} \end{pmatrix}, \quad \boldsymbol{\tau}(\mathbf{s}, h) = \begin{pmatrix} \tau_1 \\ \vdots \\ \tau_{r_2} \end{pmatrix}, \quad \mathbf{S}(\mathbf{s}) \otimes \boldsymbol{\tau}(\mathbf{s}, h) = \begin{pmatrix} S_1 \tau_1 \\ S_1 \tau_2 \\ \vdots \\ S_1 \tau_{r_2} \\ \vdots \\ S_{r_1} \tau_1 \\ S_{r_1} \tau_2 \\ \vdots \\ S_{r_1} \tau_{r_2} \end{pmatrix}.$$

- $\boldsymbol{\tau}(\mathbf{s}, h)$ expands h from one number to a vector of six numbers in a way that depends on location $\mathbf{s}$.

Modeling and exploiting spatial covariance

The data model relates each instrument footprint observed value to the true process:

$$\mathbf{Z}_t^{(k)} = \begin{pmatrix} \mathbf{Z}^{(k)}(B_{k1t}) \\ \vdots \\ \mathbf{Z}^{(k)}(B_{kN_t^{(k)}t}) \end{pmatrix}, \quad \mathbf{Z}^{(k)}(B_{kit}) = \mathbf{Y}^{(k)}(B_{kit}, t) + \epsilon(B_{kit}),$$

$$\mathbf{Y}^{(k)}(B_{kit}) = \left[\frac{1}{|D \cap B_{kit}|} \sum_{\mathbf{s} \in |D \cap B_{kit}|} \mathbf{Y}(\mathbf{s}, t) \right] \quad \text{(noiseless spatial aggregate)},$$

$$= \left[\frac{1}{|D \cap B_{kit}|} \sum_{\mathbf{s} \in |D \cap B_{kit}|} \boldsymbol{\mu}^{(k)}(\mathbf{s}, t) + \mathbf{S}(\mathbf{s})\boldsymbol{\eta}_t + \boldsymbol{\xi}^{(k)}(\mathbf{s}, t) \right].$$